

United Aircraft Research Laboratories

EAST HARTFORD, CONNECTICUT

N68-16663

FACILITY FORM 602

(ACCESSION NUMBER)

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(CODE)

(NASA CR OR TMX OR AD NUMBER)

(CATEGORY)

United Aircraft Research Laboratories



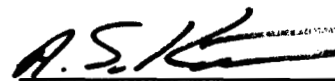
UNITED AIRCRAFT CORPORATION

EAST HARTFORD, CONNECTICUT

Report G910461-21

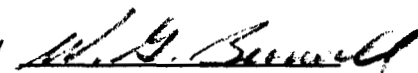
Analytical Study of Catalytic Reactors
for Hydrazine Decomposition
Quarterly Progress Report No. 6
Contract NAS 7-458

REPORTED BY



A. S. Kesten

APPROVED BY



Wayne G. Burwell, Chief
Kinetics & Thermal Sciences

DATE January, 1968

NO. OF PAGES 23

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Analytical Study of Catalytic Reactors
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Quarterly Progress Report No. 6

October 15, 1967 - January 14, 1968

Contract NAS 7-458

TABLE OF CONTENTS

	<u>Page</u>
SUMMARY	1
INTRODUCTION	2
DISCUSSION	3
REFERENCES	6
LIST OF SYMBOLS	7
FIGURES 1 through 14	10

United Aircraft Research Laboratories



Report G910461-21
Date: January 29, 1968
Prepared by: A. S. Kesten

National Aeronautics and Space Administration
NASA Resident Office
Jet Propulsion Laboratory
4800 Oak Grove Drive
Pasadena, California 91103A

Attention: Mr. James S. Evans
Contracting Officer, T-93

Subject: Analytical Study of Catalytic Reactors for Hydrazine Decomposition.
Contract NAS 7-458. Transmittal of Sixth Quarterly Progress Report
for the Period October 15, 1967 - January 14, 1968.

Enclosures: (A) Cumulative Total Expenditures
(B) Cumulative Direct Labor
(C) Revised Project Work Plan
(D) One (1) copy of the subject quarterly report

Gentlemen:

1. Enclosed herewith is one (1) copy of the sixth quarterly progress report on the work specified in Article I of the Contract Schedule. This report is being transmitted in accordance with the reporting requirements set forth in Article II.

2. Approximately 1200 manhours and \$16,800 have been expended during this report period. Enclosures A and B indicate the cumulative cost and effort, respectively. Enclosure (C) is the Revised Project Work Plan with the darkened portion of the bar chart representing completed work.

Very truly yours,

UNITED AIRCRAFT CORPORATION
Research Laboratories

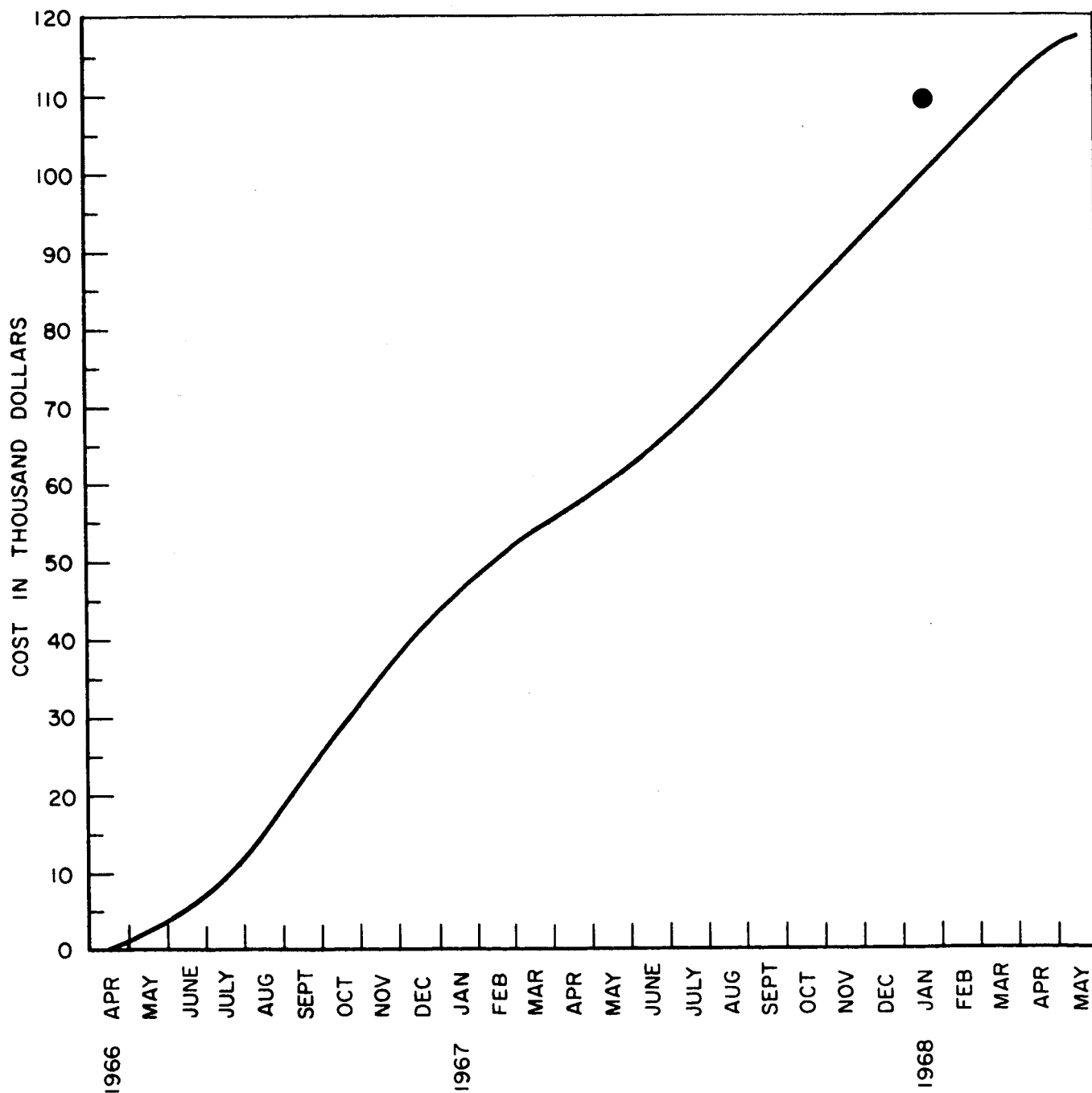
Wayne G. Burwell
Chief, Kinetics & Thermal Sciences

WGB/fap
Distributed in accordance
with attached list.

REVISED ESTIMATED PROGRESS SCHEDULE

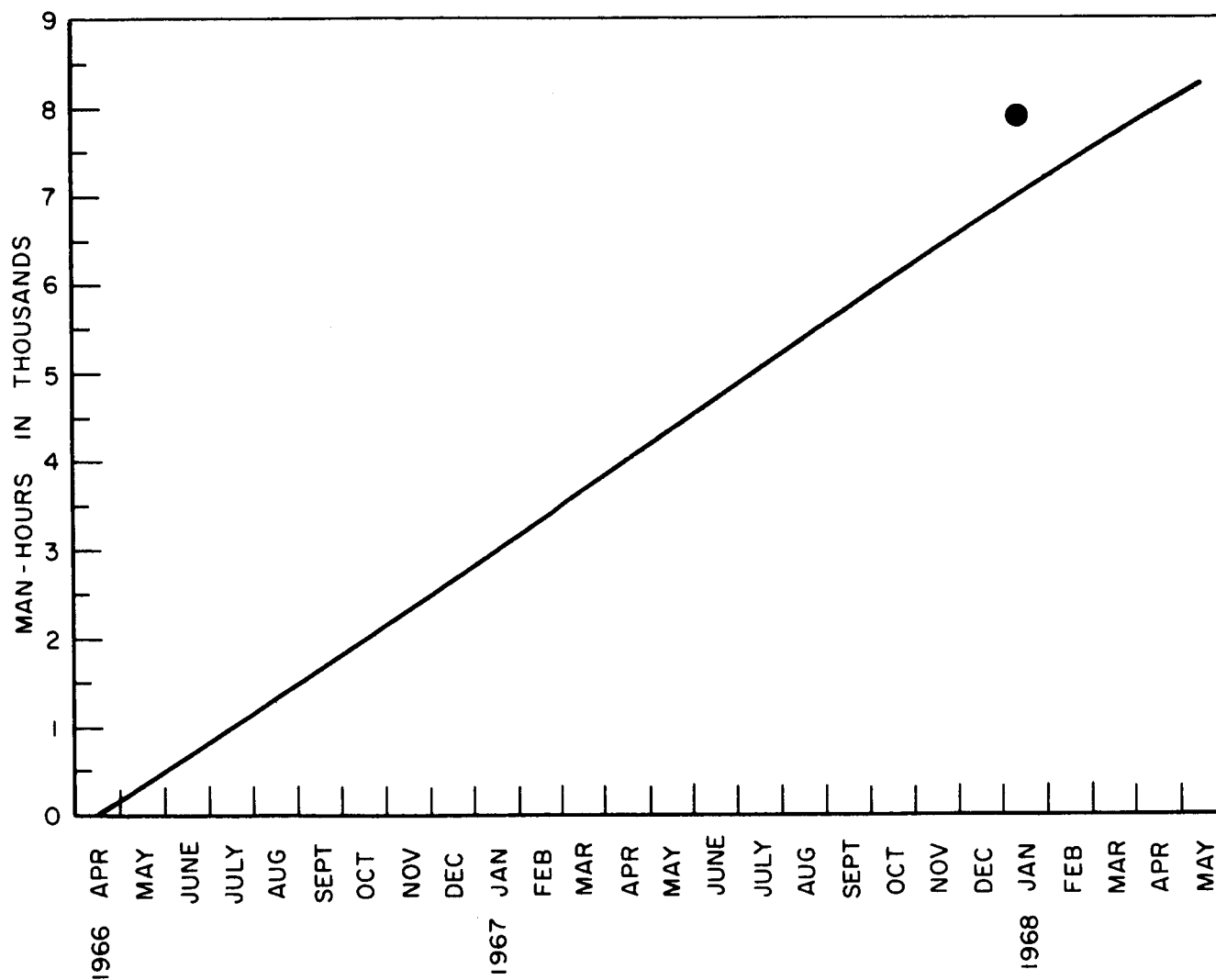
CUMULATIVE TOTAL EXPENDITURES*
NAS 7 - 458

* EXCLUSIVE OF FEE
TOTAL EXPENDITURES (DOLLARS): 117,397



REVISED ESTIMATED PROGRESS SCHEDULE
CUMULATIVE DIRECT LABOR
NAS 7 - 458

TOTAL MAN - HOURS : 8260



Report G910461-21

Analytical Study of Catalytic Reactors
for Hydrazine Decomposition

Quarterly Progress Report No. 6

October 15, 1967 - January 14, 1968

Contract NAS 7-458

SUMMARY

The Research Laboratories of United Aircraft Corporation under Contract NAS 7-458 with the National Aeronautics and Space Administration are performing an analytical study of catalytic reactors for hydrazine decomposition. This report summarizes work performed during the seventh quarterly contract period from October 15, 1967 to January 14, 1968. Work during this reporting period has included the debugging and running of the computer program representing the two-dimensional steady-state model of a distributed-feed catalyzed hydrazine decomposition reaction chamber. Calculations have been made of the effects on steady-state temperature and reactant concentration distributions of nonuniform radial injection and of catalyst bed configurations exhibiting both radial and axial nonuniformities.

Empirical predictions have been developed of one-dimensional steady-state temperature and fractional ammonia dissociation profiles in hydrazine reactors packed with Shell 405 catalyst particles. The empirical correlations were developed on the basis of many runs made with the steady-state computer program developed during the first year of effort on the present contract. It was found that fractional ammonia dissociation and bulk fluid temperature are easily predicted for a broad range of operating conditions for cases in which most of the hydrazine decomposition occurs in the first few tenths of an inch of the reactor; this rapid hydrazine decomposition rate is associated with reactors packed with particles 25 mesh or smaller for approximately 0.2 in.

INTRODUCTION

Under Contract NAS 7-458, the Research Laboratories of United Aircraft Corporation are performing analytical studies of the behavior of distributed-feed catalytic reactors for hydrazine decomposition. The specific objectives of this program are (a) to develop computer programs for predicting the temperature and concentration distributions in monopropellant hydrazine catalytic reactors in which hydrazine can be injected at arbitrary axial and radial locations in the reaction chamber and (b) to perform calculations using these computer programs to demonstrate the effects of various system parameters on the performance of the reactor.

Progress previously reported in the first three quarterly reports (Refs. 1, 2 and 3) and in the first annual report (Ref. 4) included the development of computer programs which describe the steady-state and transient behavior of a reactor system in which complete radial mixing in the free-gas (or liquid) phase was assumed. Progress described in the fourth and fifth quarterly reports (Refs. 5 and 6) included an extension of the computer program describing the steady-state model to permit radial as well as axial variations in temperature and concentrations. The program contains a description of the turbulent diffusion of heat and mass in the interstitial phase along with heat and mass diffusion within the catalyst particles and between the particles and the interstitial phase. During this reporting period attention has been focused on debugging and running the computer program representing the two-dimensional steady-state model in order to evaluate steady-state reactor behavior. In addition, the one-dimensional steady-state program has been used to develop empirical correlations which predict axial temperature and fractional ammonia dissociation profiles in hydrazine reactors packed with Shell 405 catalyst particles.

DISCUSSION

Effort during the seventh quarterly reporting period of Contract NAS 7-458 has involved (a) debugging the computer program representing the two-dimensional steady-state model, (b) running this program to evaluate the effects on steady-state temperature and reactant concentration distributions of nonuniform radial injection and of catalyst bed configurations exhibiting both radial and axial nonuniformities, and (c) using the one-dimensional program to develop empirical correlations to predict axial temperature and fractional ammonia dissociation profiles in hydrazine reactors packed with Shell 405 catalyst particles. This effort is described in detail in succeeding sections of this report.

Two-Dimensional Steady-State Program

A series of calculations was made using the two-dimensional steady-state computer program in order to examine the effectiveness of the two-dimensional model and to evaluate the effects on system performance of nonuniform radial injection and of catalyst bed configurations exhibiting both radial and axial nonuniformities. The calculated results illustrated in Figs. 1 through 12 refer to a reactor 3 in. in diameter into which liquid hydrazine is injected at the upstream end of the reactor only. For these calculations the upstream chamber pressure was taken as 100 psia and the hydrazine feed temperature was taken as 530 deg R.

Axial temperature profiles at various radial locations are plotted in Fig. 1 for a case in which a radial nonuniformity in mass flow rate, G , is represented as a step function (see Fig. 1). In this case the catalyst bed packing was taken to consist of 25-30 mesh catalyst particles for the first 0.2 in. and 1/8 in. x 1/8 in. cylindrical pellets for the remainder of the bed. This configuration is referred to in the figures as the "standard bed configuration". Turbulent diffusion of heat, which tends to reduce radial temperature gradients, is more pronounced in the downstream end of the reactor. Here the catalyst particle size is larger, and both eddy conductivity and eddy diffusivity are directly proportional to particle size. The consequences of radial heat conduction are complicated somewhat by the simultaneous turbulent diffusion of mass. Higher temperatures are associated with more hydrazine decomposition; thus high temperature regions may lose heat by radial conduction, but may gain hydrazine from adjoining low temperature regions by radial diffusion of mass. Subsequent decomposition of this hydrazine may lead to even higher temperatures. For the case considered here, these combined effects lead to the temperature distribution shown in Fig. 1. For comparison purposes, the axial temperature profile corresponding to a radially uniform mass flow rate of 3.0 lb/ft²-sec is also plotted in Fig. 1. This is the average mass flow rate calculated by averaging the actual mass flow rate profile over the cross-

sectional area of the reactor. The mole-fraction distributions of hydrazine and ammonia associated with the temperature distribution shown in Fig. 1 are illustrated in Figs. 2 and 3 respectively.

The results of similar calculations made for a continuously varying injection profile are shown in Figs. 4 through 6. The mass flow rate profile used for these calculations is plotted in Fig. 3. As in the first set of calculations, the average mass flow rate is 3.0 lb/ft²-sec.

The effects on temperature and reactant concentration distributions of two catalyst bed configurations exhibiting both radial and axial nonuniformities are illustrated in Figs. 7 through 12. For both of these configurations the mass flow rate was taken as uniform at 3.0 lb/ft²-sec. The calculated temperature, mole fraction of hydrazine, and mole fraction of ammonia distributions corresponding to the bed configuration shown in Fig. 7 are plotted in Figs. 7 through 9 respectively. Similar calculations corresponding to the bed configuration shown in Fig. 10 are plotted in Figs. 10 through 12.

One-Dimensional Steady-State Program

A series of runs were made with the one-dimensional steady-state computer program in order to develop empirical correlations to predict axial temperature and fractional ammonia dissociation profiles in hydrazine reactors packed with Shell 405 catalyst particles. Empirical correlations were developed on the basis of about 65 runs representing different combinations of mass flow rates, pressures and catalyst bed configurations. It was found that fractional ammonia dissociation and bulk fluid temperature can be predicted using the equations

$$I - \text{Fractional Ammonia Dissociation} = \Phi$$

and

$$T_i = 1020 \left\{ \Phi + [0.075 (P/1000)] \right\} + 1535$$

where

$$\Phi = (0.66) (G/z)^{0.28} \left\{ [(0.55 a^{0.17} - 0.17) (1000/P)^{0.22}] + 0.17 \right\}$$

and z and a are expressed in ft, G in lb/ft²-sec, P in psia, and T_i in deg R.

These equations are illustrated in Figs. 13 and 14 respectively for cases in which most of the hydrazine decomposition occurs in the first few tenths of an inch of the reactor; this rapid hydrazine decomposition rate is associated with reactors packed with particles 25 mesh or smaller for approximately 0.2 in. For these cases the correlations depicted in Figs. 13 and 14 work well for axial distances greater than one inch and for values of pressure, P , between 10 and 1000 psia, mass flow rate, G , between 1.44 and 14.4 lb/ft²-sec (0.01 and 0.1 lb/in.²-sec respectively) and equivalent spherical radius, a , between 0.001 and 0.01 ft. For a reactor packed with small (≤ 25 mesh) particles for the first few tenths of an inch and larger particles thereafter, the particle radius, a , refers to the larger particles.

In Figs. 13 and 14, Rocket Research experimental data are plotted along with the empirical predictions and the results of sample cases run using the one-dimensional steady-state program. Values of fractional ammonia dissociation obtained from the steady-state program are plotted for axial locations between 1 and 6 inches while values of bulk fluid temperature obtained from the program are plotted only for axial locations between 3 and 6 inches.

It should be emphasized that these empirical correlations do not correctly predict the behavior of reactors in which hydrazine decomposition is slow, for example reactors which are uniformly packed with large catalyst particles, such as 1/8 in. x 1/8 in. cylinders. The correlations work quite well though for catalyst bed configurations consisting of 25-30 mesh particles for the first 0.2 in. and 1/8 in. x 1/8 in. cylindrical pellets for the remainder of the bed.

REFERENCES

1. Kesten, A. S.: Analytical Study of Catalytic Reactors for Hydrazine Decomposition. United Aircraft Research Laboratories Report E910461-3, Quarterly Progress Report No. 1, Contract NAS 7-458, July 1966.
2. Kesten, A. S.: Analytical Study of Catalytic Reactors for Hydrazine Decomposition. United Aircraft Research Laboratories Report E910461-6, Quarterly Progress Report No. 2, Contract NAS 7-458, October 1966.
3. Kesten, A. S.: Analytical Study of Catalytic Reactors for Hydrazine Decomposition. United Aircraft Research Laboratories Report F910461-9, Quarterly Progress Report No. 3, Contract NAS 7-458, January 1967.
4. Kesten, A. S.: Analytical Study of Catalytic Reactors for Hydrazine Decomposition. United Aircraft Research Laboratories Report F910461-12, First Annual Progress Report, Contract NAS 7-458, July 1967.
5. Kesten, A. S.: Analytical Study of Catalytic Reactors for Hydrazine Decomposition. United Aircraft Research Laboratories Report F910461-15, Quarterly Progress Report No. 4, Contract NAS 7-458, July 1967.
6. Kesten, A. S.: Analytical Study of Catalytic Reactors for Hydrazine Decomposition. United Aircraft Research Laboratories Report F910461-18, Quarterly Progress Report No. 5, Contract NAS 7-458, October 1967.

LIST OF SYMBOLS

a	Radius of spherical particle, ft
A_p	Total external surface of catalyst particle per unit volume of bed, ft^{-1}
c_i	Reactant concentration in interstitial fluid, lb/ft^3
c_p	Reactant concentration in gas phase within the porous particle, lb/ft^3
c_p^*	Equals $c_p - (c_p)_s$, lb/ft^3
C_F	Specific heat of fluid in the interstitial phase, $\text{Btu}/\text{lb} - \text{deg R}$
\bar{C}_F	Average specific heat of fluid in the interstitial phase, $\text{Btu}/\text{lb} - \text{deg R}$
C_s	Specific heat of catalyst particle, $\text{Btu}/\text{lb} - \text{deg R}$
D_i	Diffusion coefficient of reactant gas in the interstitial fluid, ft^2/sec
D_p	Diffusion coefficient of reactant gas in the porous particle, ft^2/sec
F	Rate of feed of hydrazine from distributed injectors into the system, $\text{lb}/\text{ft}^3\text{-sec}$
g_c	Conversion factor, $(\text{lb}_m/\text{lb}_f) \text{ft}/\text{sec}^2$
G	Mass flow rate, $\text{lb}/\text{ft}^2\text{-sec}$
h	Enthalpy, Btu/lb
h_c	Heat transfer coefficient, $\text{Btu}/\text{ft}^2\text{-sec-deg R}$
H	Heat of reaction (negative for exothermic reaction), Btu/lb
k_c	Mass transfer coefficient, ft/sec
k_0	Reaction rate constant, equals $a e^{-\gamma}$, sec^{-1}
K_p	Thermal conductivity of the porous catalyst particle, $\text{Btu}/\text{ft-sec-deg R}$
M	Molecular weight, $\text{lb}/\text{lb mole}$
\bar{M}	Average molecular weight, $\text{lb}/\text{lb mole}$

n	Order of decomposition reaction
P	Chamber pressure, psia
Q	Activation energy, Btu/lb mole
r	Radial distance, ft
r_{het}	Rate of (heterogeneous) chemical reaction on the catalyst surfaces, lb/ft ³ -sec
r_{hom}	Rate of (homogeneous) chemical reaction in the interstitial phase, lb/ft ³ -sec
R	Gas constant, equals 10.73 psia - ft ³ /lb mole - deg R, or, Radius of reactor
t	Time, sec
t^*	Actual time minus time required, under steady-state conditions, for liquid hydrazine to flow from the reactor inlet to the interface between the liquid-vapor and vapor regions, sec
T	Temperature, deg R
w_i	Weight fraction of reactant in interstitial phase
x	Radial distance from the center of the spherical catalyst particle, ft
z	Axial distance, ft
α	Preexponential factor in rate equation
α_p	Intraparticle void fraction
β	Equals $\left[- (C_P)_S H D_P \right] / \left[K_P (T_P)_S \right]$
γ	Equals $Q / R (T_P)_S$
δ	Interparticle void fraction
ϵ	Eddy diffusivity, ft ² /sec
λ	Eddy conductivity, Btu/ft-sec-deg R

μ Viscosity of interstitial fluid, lb/ft - sec

ρ_i Density of interstitial fluid, lb/ft³

ρ_s Bulk density of catalyst particle, lb/ft³

Subscripts

F Refers to feed

i Refers to interstitial phase

j Axial distance index in transient model

P Refers to gas within the porous catalyst particle

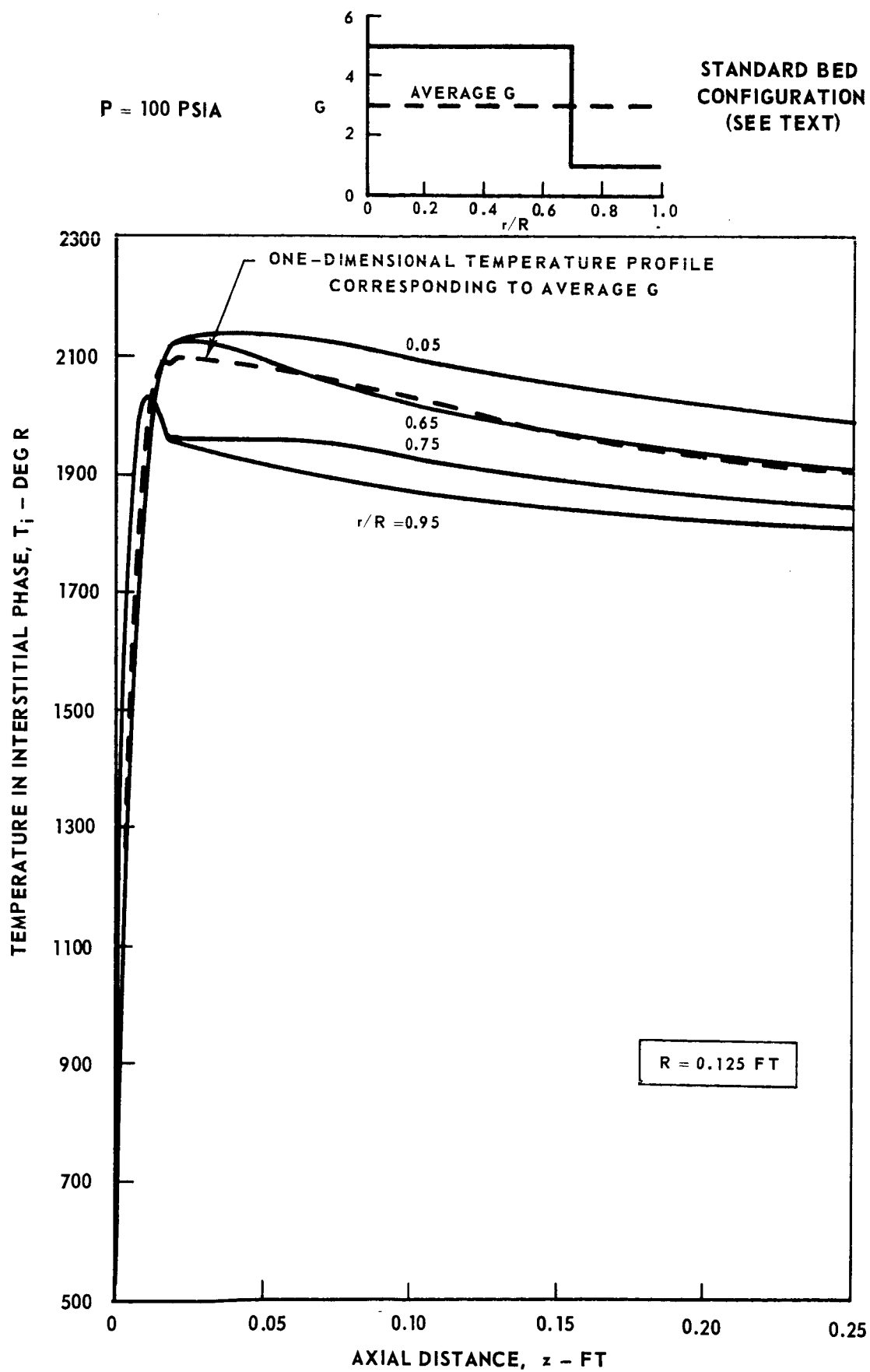
s Refers to surface of catalyst particle

Superscripts

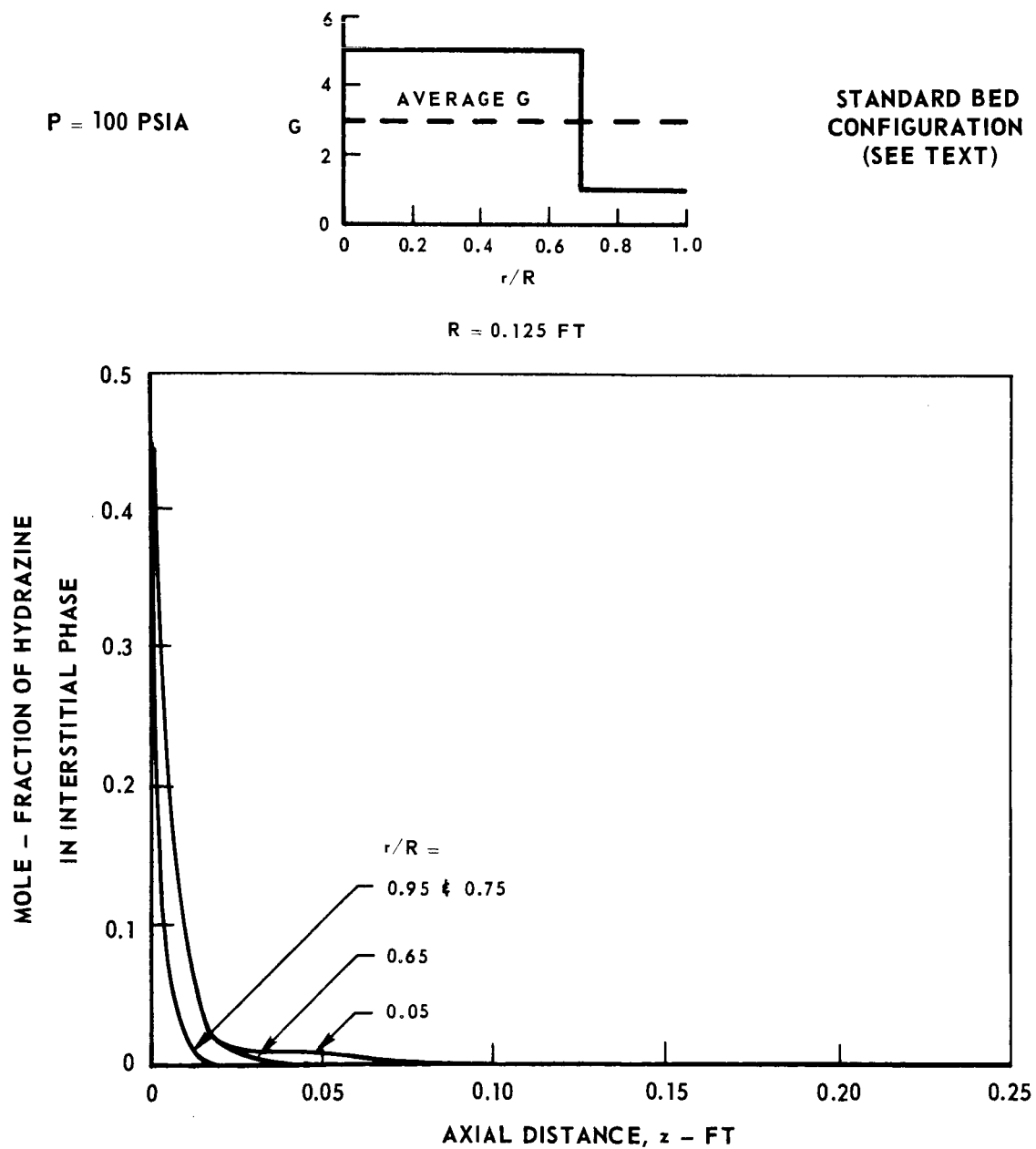
J Refers to chemical species

L Refers to liquid at vaporization temperature

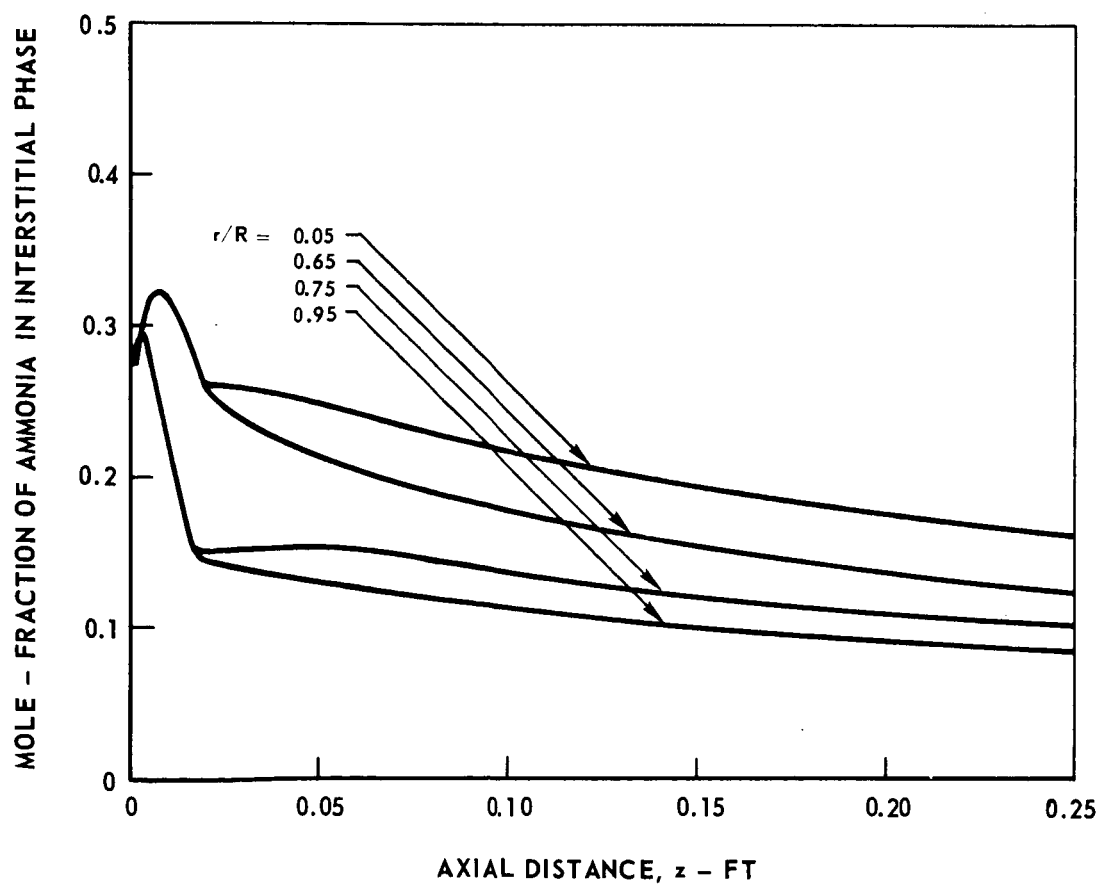
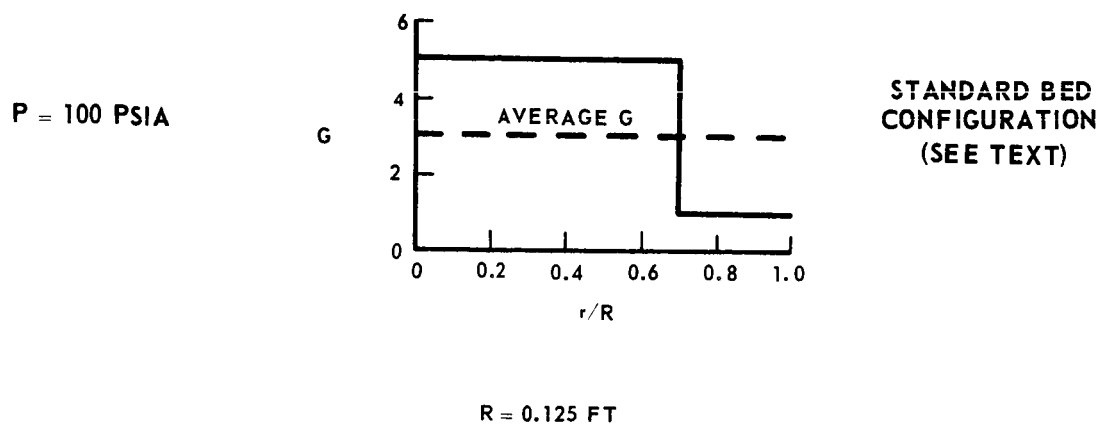
V Refers to vapor at vaporization temperature

TWO - DIMENSIONAL STEADY - STATE
TEMPERATURE DISTRIBUTION

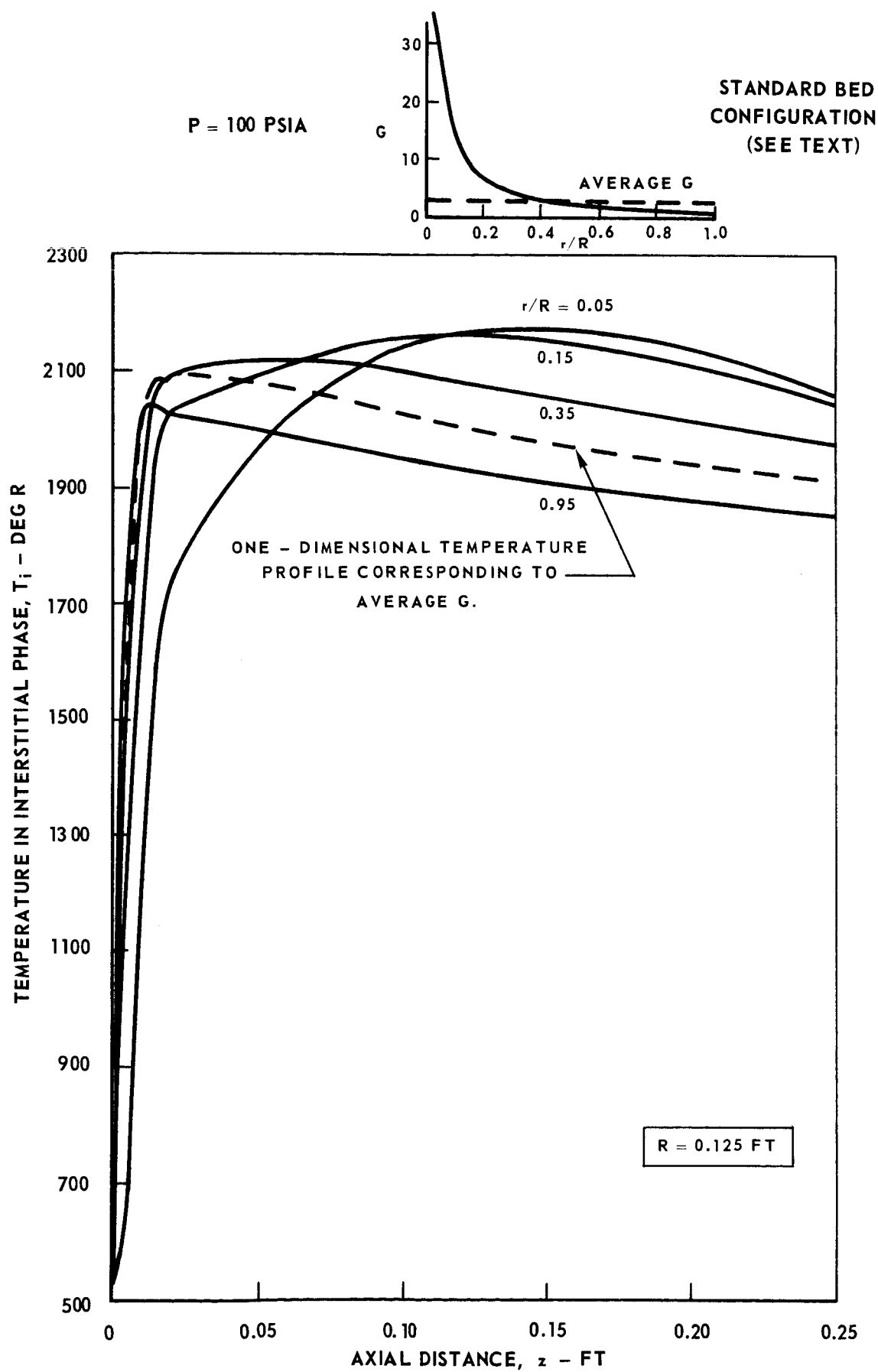
TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION
OF MOLE - FRACTION OF HYDRAZINE

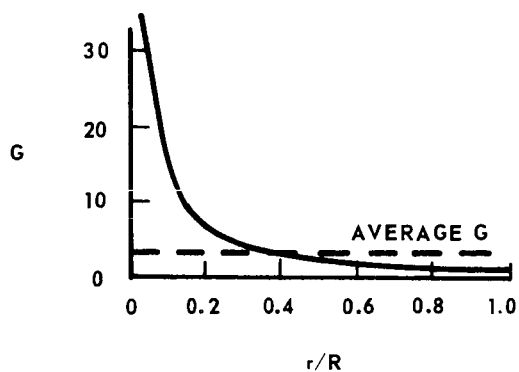
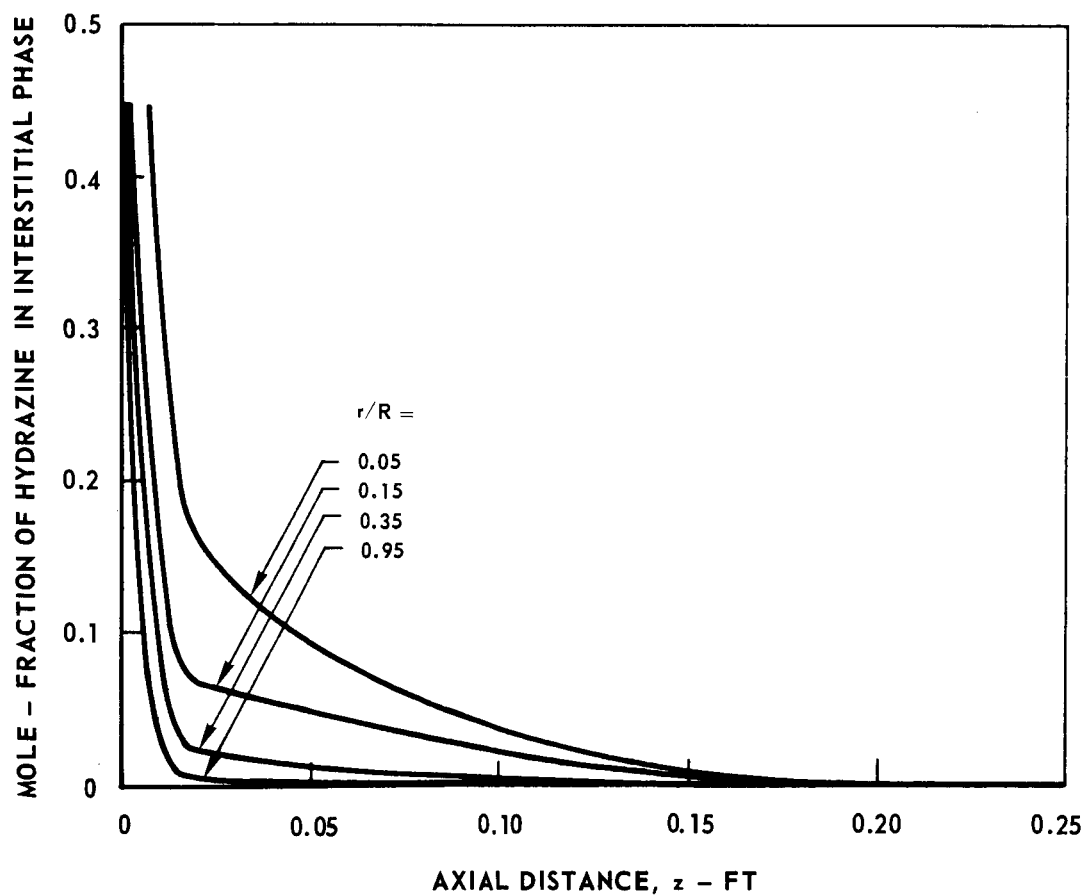


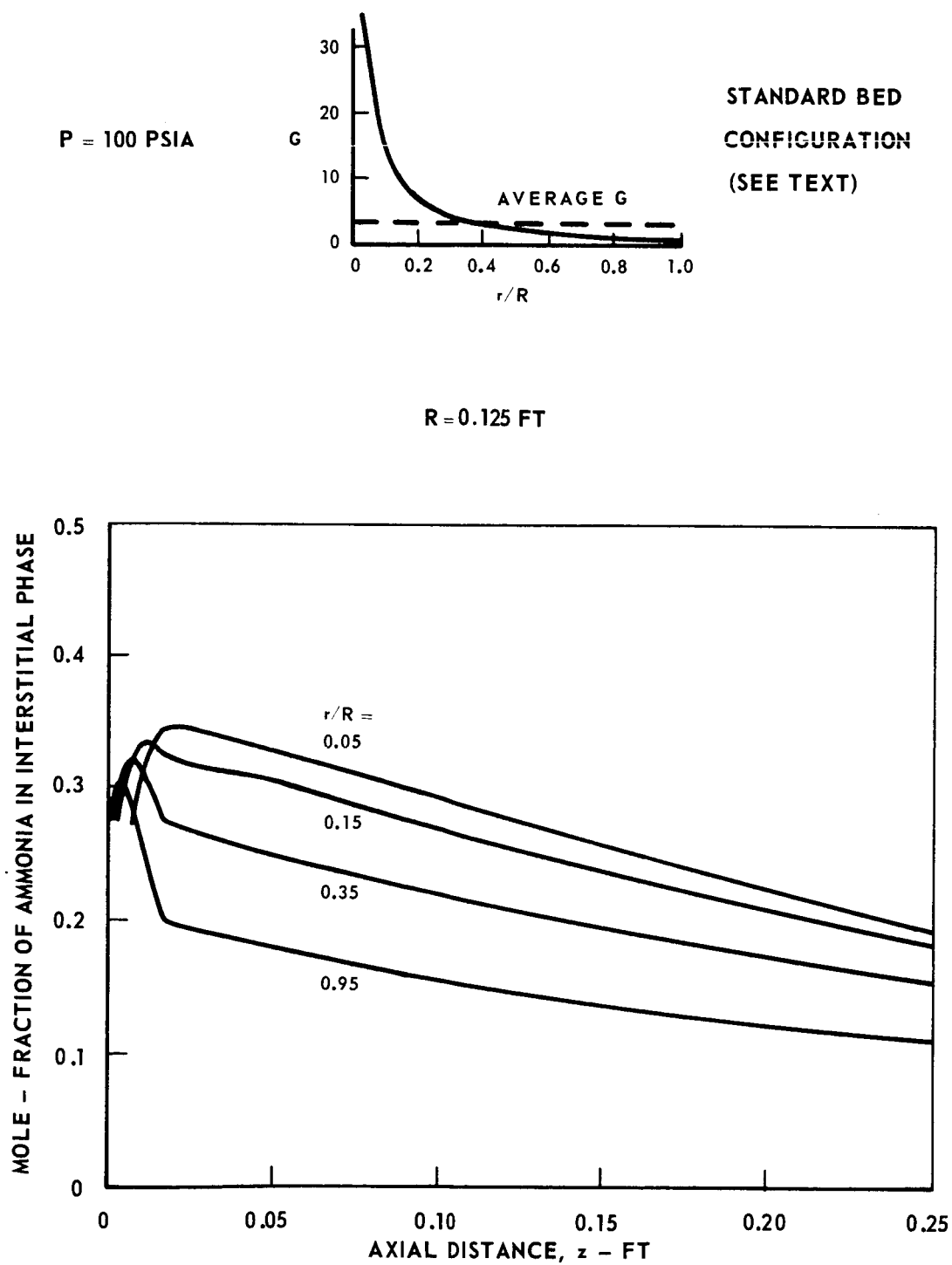
TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION OF MOLE - FRACTION OF AMMONIA



TWO - DIMENSIONAL STEADY - STATE TEMPERATURE DISTRIBUTION



TWO - DIMENSIONEL STEADY - STATE DISTRIBUTION
OF MOLE - FRACTION OF HYDRAZINE $P = 100 \text{ PSIA}$ STANDARD BED
CONFIGURATION
(SEE TEXT) $R = 0.125 \text{ FT}$ 

TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION
OF MOLE - FRACTION OF AMMONIA

TWO - DIMENSIONAL STEADY - STATE TEMPERATURE DISTRIBUTION

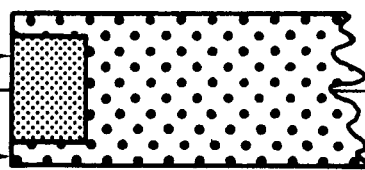
 $P = 100 \text{ PSIA}$ $G = 3.0 \text{ LB/FT}^2 - \text{SEC}$

CATALYST BED CONFIGURATION:

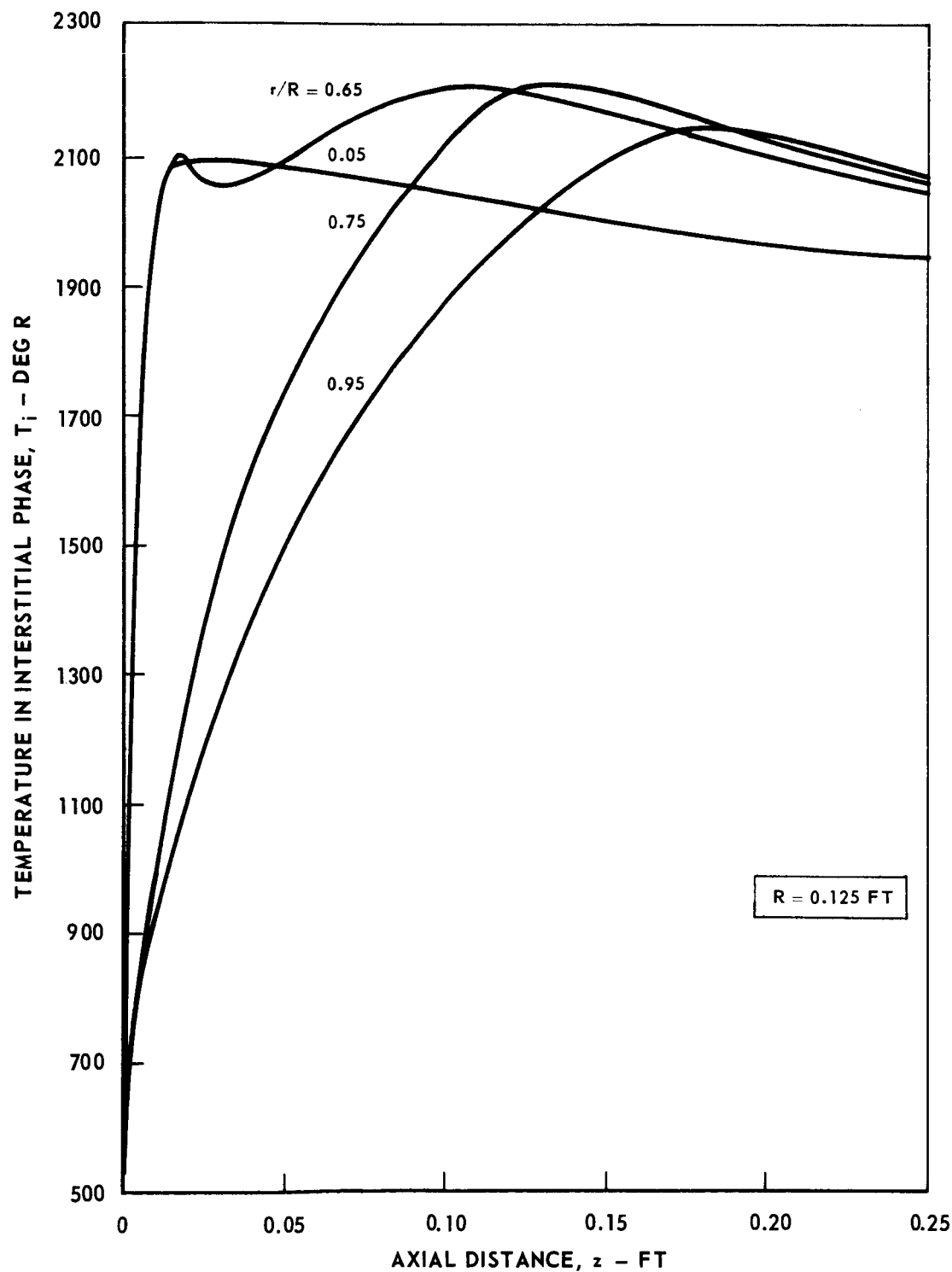
ALL 25 - 30 MESH
GRANULES

ALL 1/8" x 1/8"

CYLINDRICAL PELLETS



0.0167 FT

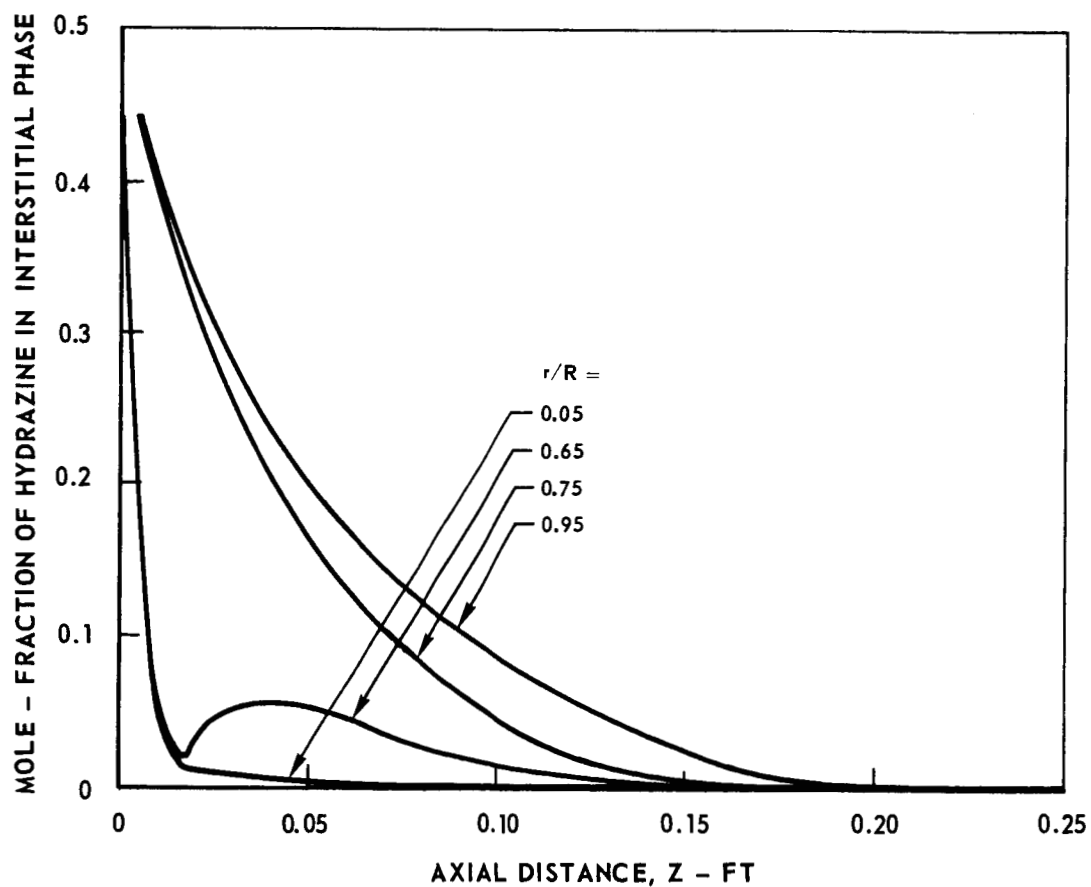
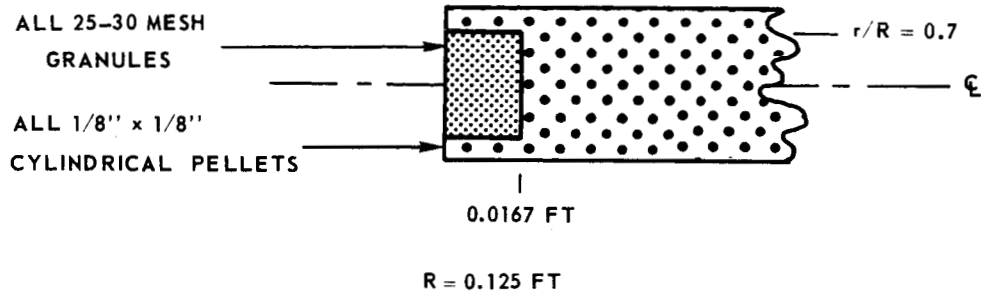


TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION OF MOLE - FRACTION OF HYDRAZINE

P = 100 PSIA

G = 3.0 LB/FT² - SEC

CATALYST BED CONFIGURATION:

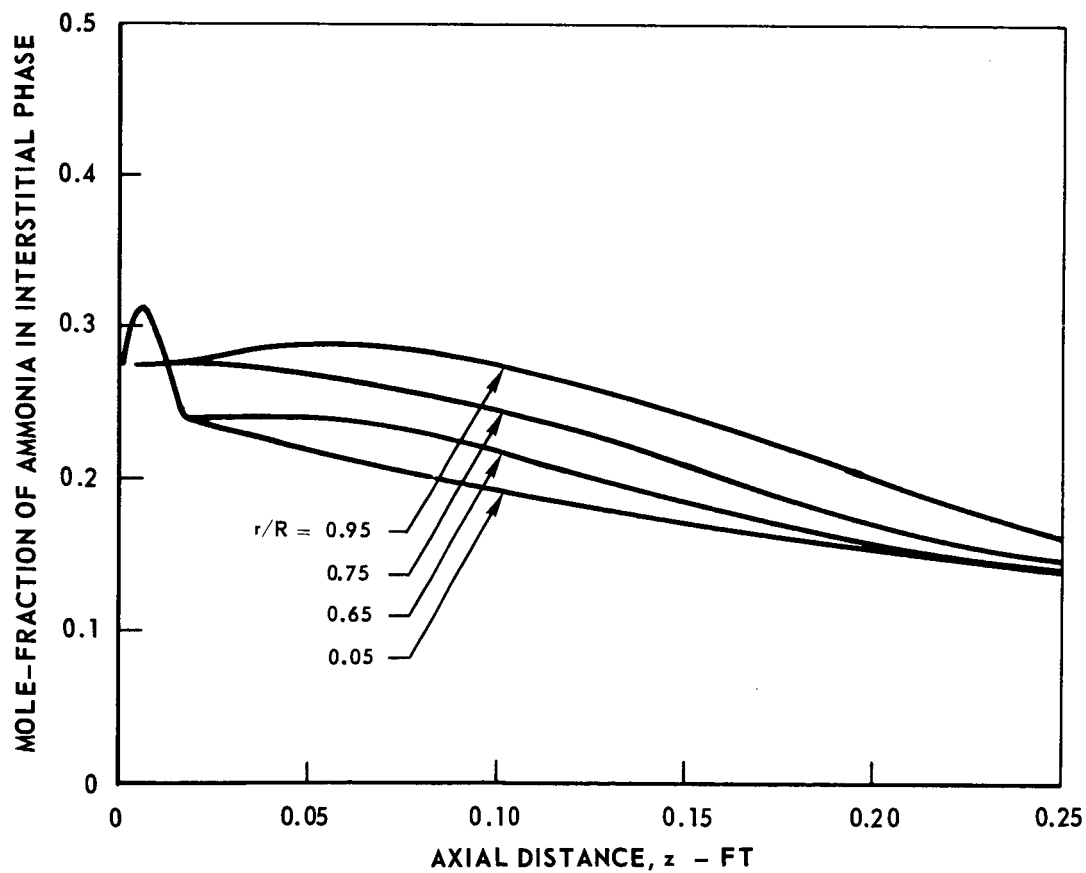
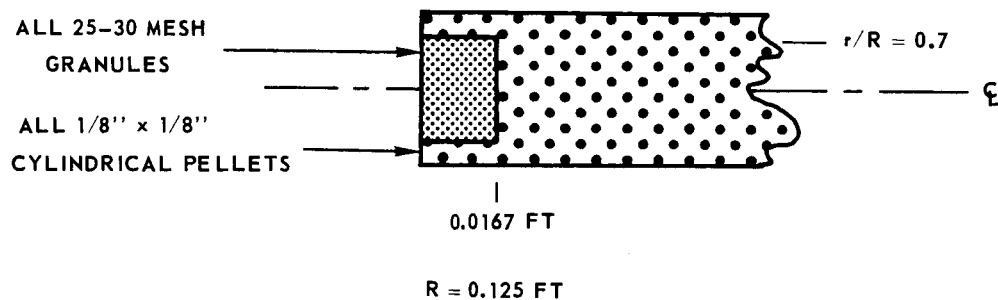


TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION OF MOLE - FRACTION OF AMMONIA

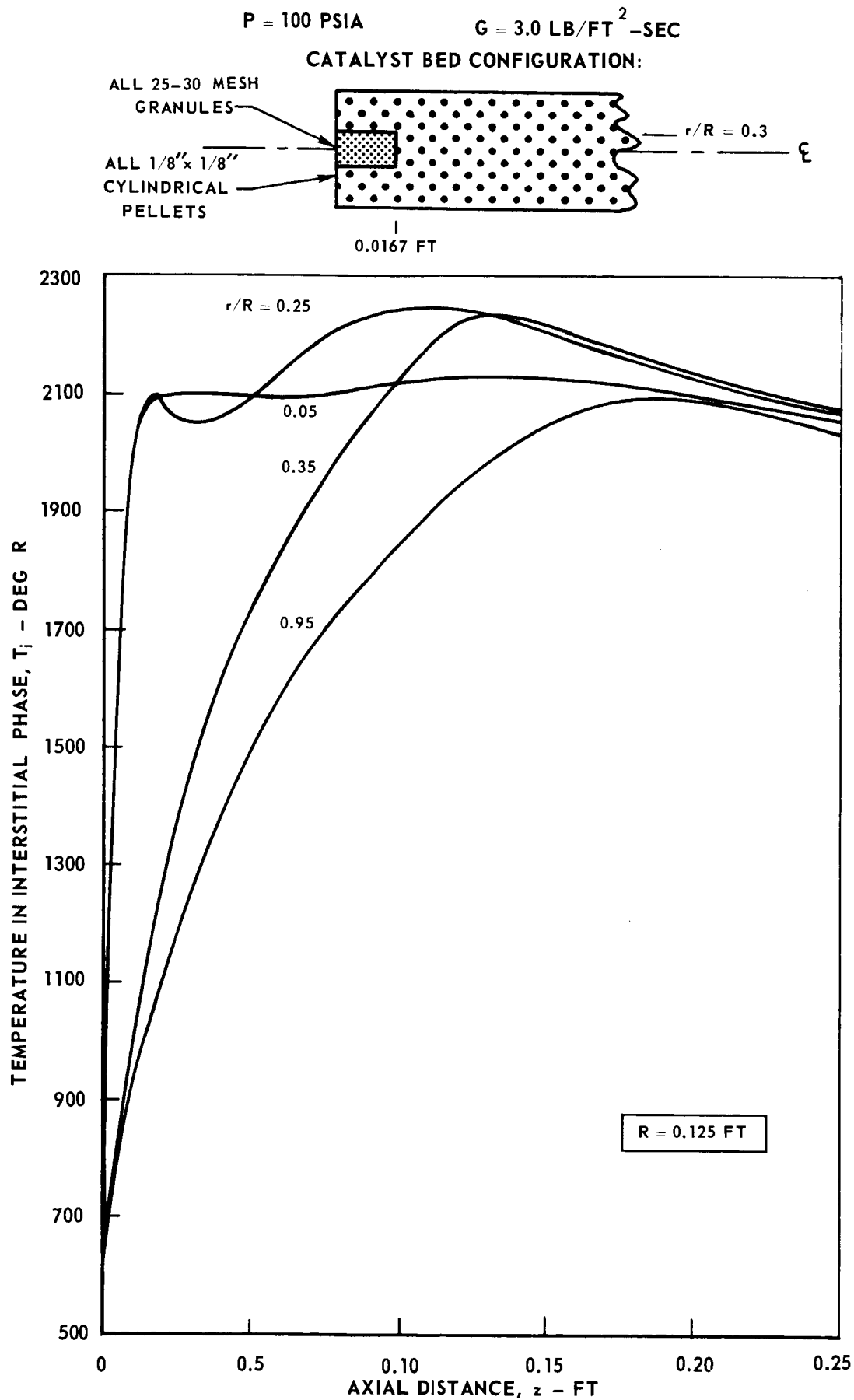
$P = 100 \text{ PSIA}$

$G = 3.0 \text{ LB/FT}^2 \text{ -SEC}$

CATALYST BED CONFIGURATION:



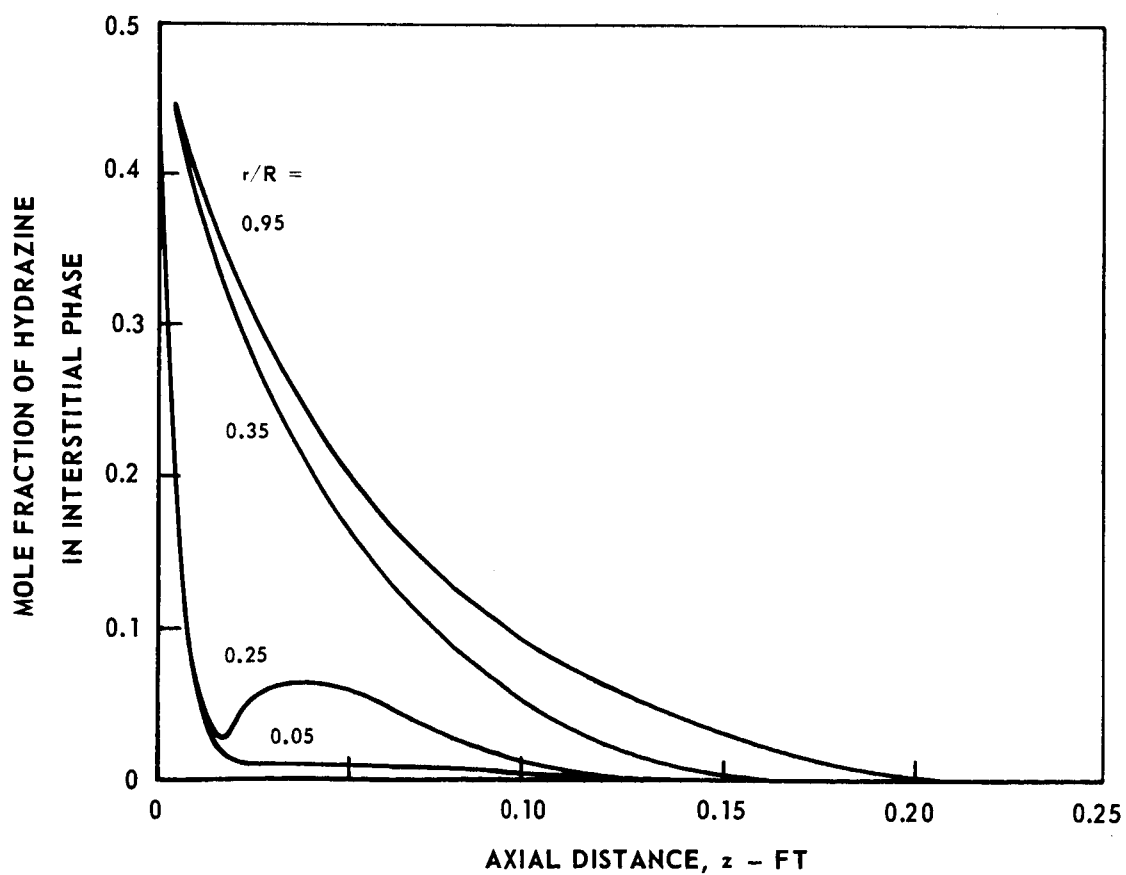
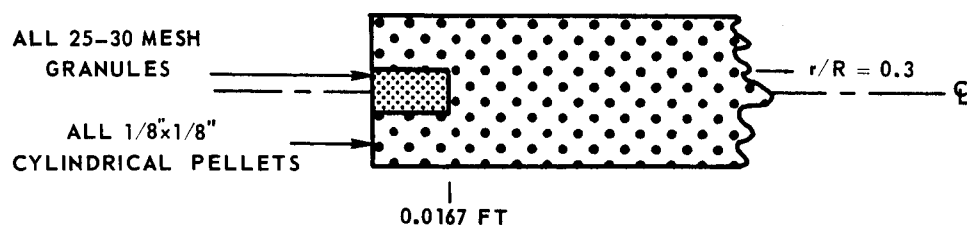
TWO - DIMENSIONAL STEADY - STATE TEMPERATURE DISTRIBUTION



TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION OF MOLE - FRACTION OF HYDRAZINE

$$P = 100 \text{ PSIA} \quad G = 3.0 \text{ LB/FT}^2 - \text{SEC}$$

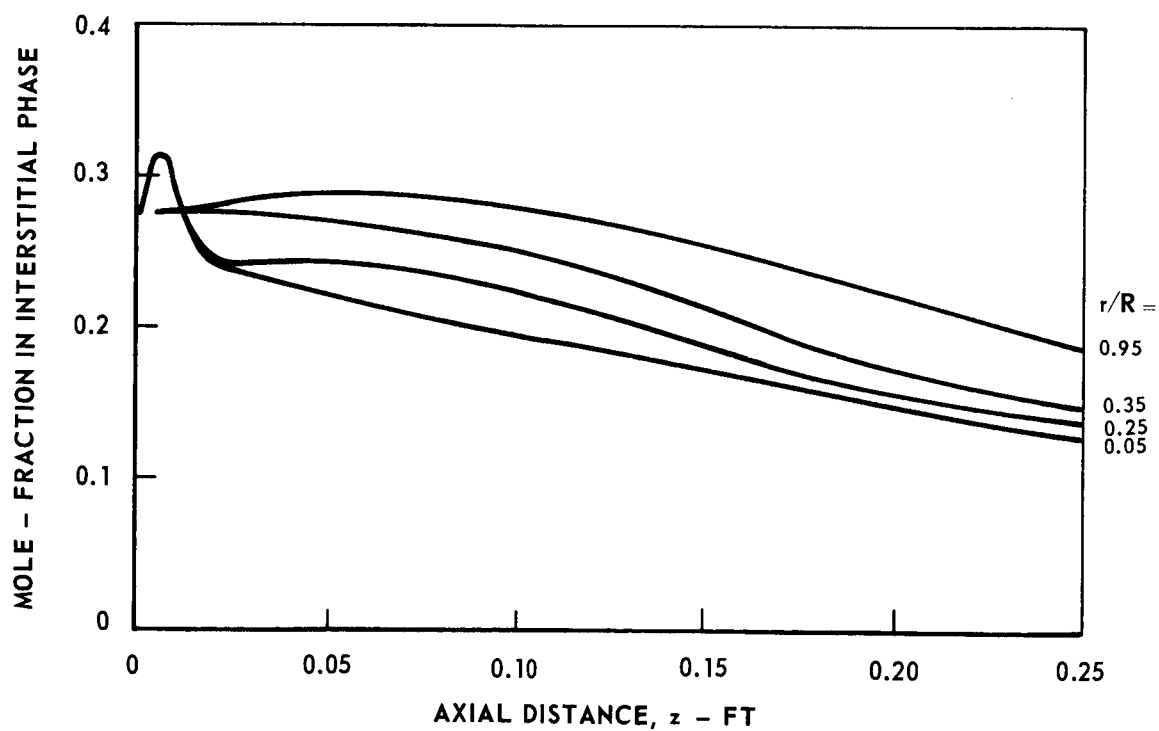
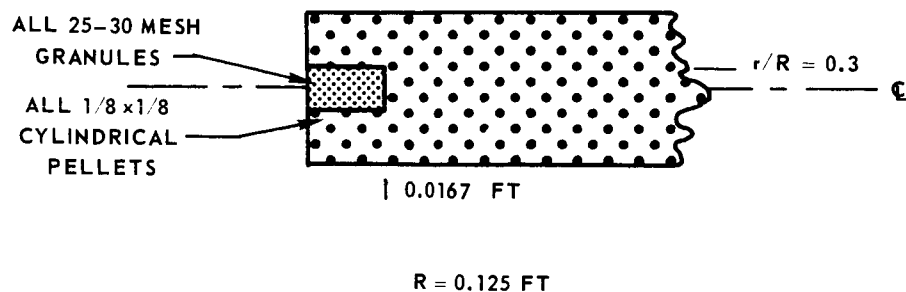
CATALYST BED CONFIGURATION:



TWO - DIMENSIONAL STEADY - STATE DISTRIBUTION OF MOLE - FRACTION OF AMMONIA

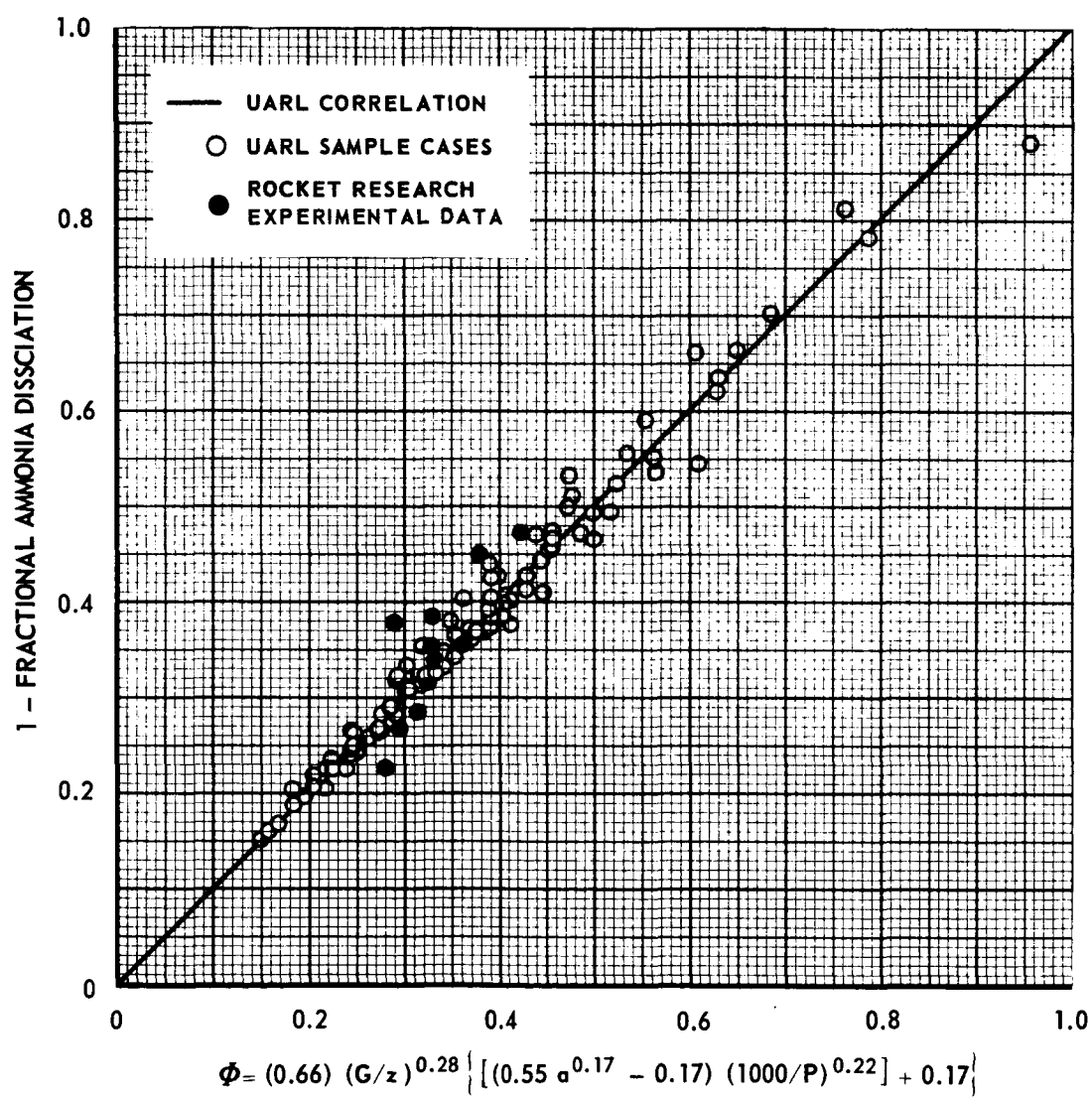
 $P = 100 \text{ PSIA}$ $G = 3.0 \text{ LB/FT}^2 - \text{SEC}$

CATALYST BED CONFIGURATION:



EMPIRICAL PREDICATION OF FRACTIONAL AMMONIA DISSOCIATION

SYMBOL	UNITS
z	FT
G	LB/FT ² -SEC
P	PSIA
a	FT



EMPIRICAL PREDICTION OF INTERSTITIAL
GAS TEMPERATURE

SYMBOL	UNITS
P	PSIA
$T_i(z)$	DEG R

